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GENERALIZED CONTINUOUS SLOWING-DOWN THEORY

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ABSTRACT

Continuous slowing-down theory is generalized so that inelastic scattering can be taken into account accurately.

The basic idea underlying generalized theory is the assumption that the ratio R(u), of the solution spectrum to a reference spectrum, g(u), varies linearly with the lethargy, u; that is, R(u) can be approximated by two terms of a Taylor's series as long as g(u) is chosen reasonably. Such conventional theories as Geortzel-Greuling (GG) or Stacey's Improved-GG (I-GG) are included in this theory by taking g(u) as $1/\Sigma_{s,i}(u)$ or $1/\Sigma_t(u)$, respectively.

The present theory is demonstrated to yield quite accurate results for the neutron spectra and coarse-group effective cross sections in many varieties of core and blanket compositions of fast reactors, using three alternative prescriptions for g(u).

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I. INTRODUCTION

Much work has been done on the application of the continuous slowing-down (CSD) theory to fast-reactor spectrum calculations. The basic ideas of CSD theory were worked out[1-4] many years ago by Fermi, Wigner, Goertzel and Greuling (GG), Hurwitz and Zweifel, Amster, and others. Their methods depended upon the assumption that the isotopic scattering collision density $\Sigma_{sj}\phi(u)$ was constant (Fermi, Wigner) or linearly varying (GG) within a scattering interval, where Σ_{sj} and $\phi(u)$ are the scattering cross section of isotope j and the neutron spectrum, respectively.

However, it is clear that the above approximation will fail in situations where the inherent assumption is invalid. One difficulty occurs in the treatment of sharp resonances in a mixture of several moderating materials. When a resonance in one isotope is narrow relative to the scattering interval Δu_j of other isotopes j in the mixture, the $\Sigma_{sj}(u)\phi(u)$ is no longer linear over the scattering interval Δu_j. Another difficulty encountered in the above approximation is in the treatment of inelastic events, since the lethargy increase in inelastic scattering is so large that the linear expansion of the scattering collision density is a poor approximation.

In order to overcome the first difficulty, Stacey[5] has proposed the Improved Goertzel-Greuling (I-GG) approximation for the treatment of elastic moderation of neutrons, and successfully demonstrated its usefulness for spectrum calculation in fast-reactor compositions. To derive the I-GG equations Stacey expands the total collision density, instead of the scattering density, in a Taylor series. His approach still requires, however,

that inelastic scattering be treated by multigroup methods, since a linear expansion of the collision density is still inadequate over the large lethargy intervals involved in inelastic scattering events.

On the other hand, efforts have been made by many authors to modify CSD theory to include inelastic events and to apply their CSD theory to fast-reactor spectrum calculations. Among them, Segev[6] applied Taylor's expansion to the inelastic scattering source integral to arrive at an analog of the GG approximation for elastic scattering. The spectrum obtained by use of Segev's model does not agree well with multigroup (MG) results, probably because he retains only two terms in the series expansion of the isotopic collision density.

Dunn and Becker[7] avoided the Taylor's expansion by the introduction of a moderating parameter, $\xi(u)$, adjusted to give the correct solution in the case of zero absorption. Using this method they compute spectra in good agreement with MG spectra. However, in the Dunn and Becker method, the treatment of $\gamma(u)$, one of the two GG parameters, is somewhat arbitrary. Therefore, from a theoretical point of view, it is not clear that their definition of $\gamma(u)$ will be generally satisfactory, in spite of the good results which Dunn and Becker obtained in their tests.

Yamamoto and Ito[8] introduced an improvement by using Taylor's expansion of an approximate slowing-down density, $\xi(u)\Sigma_s(u)\phi(u)$, instead of the collision density. In the theory, fission source is replaced by fictitious inelastic scattering from a monoenergetic source in order to maintain the slowing-down density nearly constant even in the fission source range. In the Yamamoto and Ito method $\xi(u)$ is computed by solving multigroup equations very similar to the MG slowing-down equations. Therefore,

it seems reasonable to expect that computing time for the Yamamoto and Ito method will be comparable to conventional MG computing times.

Rocca-Volmerange[9] has also attacked this problem, extending the idea of Cadlihac and Pujol[10] to represent the scattering kernel $\bar{P}$ as a sum of separable kernels. The author introduced the generalized scattering sources $\psi(u,w)$ defined as

$$\psi(u,w) = \sum_i \int_{-\infty}^{u} du' \, \Sigma_{s,i}(u')\phi(u')\bar{P}_i(u' \to u + w) ,$$

and the slowing-down densities q_m defined as the m-*th* moment in w of $\psi(u,w)$. Parameters which relate the $\psi(u,0)$ and the $q_m(u)$ are determined by use of a set of N reference spectra. The relation thus obtained, and an N-*th* order differential equation for $q_m(u)$ (arising from neutron balance), are coupled and solved for the particular problem. Calculations performed for fast-reactor compositions give fairly good results using three or four reference spectra. At this time it is not yet possible to come to any conclusion as to the advantages and disadvantages of the Rocca-Volmerange method,[9] as compared with the method proposed here.

Lately Yamamura and Sekiya[11] redefined $\xi(u)$ so that the differential equation for q reduces to a Wigner-type slowing-down equation, without making any Taylor's expansions. In the application of their method to actual systems, they compute $\xi(u)$ iteratively, starting from the ordinary moderating parameter of the original Wigner approximation. Their spectra agree very well with MG spectra at the third iteration on $\xi(u)$. However, Yamamura and Sekiya do not define microscopic moderating parameters based on this method. The unavailability of such parameters reduces the advantage of their CSD theory relative to MG approximation methods.

In the present paper, the author has generalized GG and I-GG theories so that inelastic events can be taken into account accurately by using a Taylor's expansion of the ratio of the solution spectrum to a reference spectrum, g(u). The ratio will be slowly varying over the slowing-down interval as long as a reasonable g(u) is chosen. The applicability of the present method is examined through several demonstrations for many varieties of fast-reactor compositions, and consideration is given to the utilization of a microscopic moderating paramter library obtained, by the present method, in a reference composition. In the final part of the paper, the coarse-group effective cross sections (for groups of lethargy width equal to one) are compared with MG results in order to assess the accuracy of the proposed method.

II. FORMULATION

The fundamental equation for neutron balance in an infinite homogeneous medium with isotropic scattering is

$$\left[\Sigma_s(u) + \Sigma_a(u)\right]\phi(u) = \sum_i \int_{u-\Delta_i}^{u} du' \, \Sigma_{s,i}(u')\phi(u')f_i(u',u) + S(u) \quad , \quad (1)$$

where the neutron source term S(u) is

$$S(u) = \sum_i \left[\chi_{fis,i}(u) \int_0^{\infty} du' \, \nu\Sigma_{f,i}(u')\phi(u')\right] + S_{external}(u) \quad ,$$

and Δ_i stands for the maximum lethargy increase by inelastic and elastic scatterings in isotope i. The summation is over all isotopes present, and the scattering cross section $\Sigma_{s,i}(u)$ is

$$\Sigma_{s,i}(u) = \Sigma_{e,i}(u) + \Sigma_{in,i}(u) ,$$

while $f_i(u',u)$ is the scattering energy transfer kernel of isotope i:

$$f_i(u',u) = \frac{1}{\Sigma_{s,i}(u')} \left\{ \Sigma_{e,i}(u') f_{e,i}(u' \to u) + \Sigma_{in,i}(u') f_{in,i}(u' \to u) \right\} . \quad (2)$$

The neutron leakage from a system can be taken into account by adding $B_g^2/3\Sigma_{tr}(u)$ to the macroscopic absorption cross section. The subscripts a, f, e, in, and tr refer to absorption, fission, elastic, and inelastic scattering and transport, respectively, and B_g^2 stands for the buckling.

The slowing-down density is defined as

$$q(u) = \sum_i \int_{u-\Delta_i}^{u} du' \int_{u}^{u'+\Delta_i} \Sigma_{s,i}(u') \phi(u') f_i(u' \to u'') \, du'' . \quad (3)$$

Using the identity

$$\frac{dq(u)}{du} = \Sigma_s(u)\phi(u) - \sum_i \int_{u-\Delta_i}^{u} du' \, \Sigma_{s,i}(u') \phi(u') f_i(u' \to u) . \quad (4)$$

Equation (1) can be written

$$\frac{dq(u)}{du} = S(u) - \Sigma_a(u)\phi(u) . \quad (5)$$

Up to this point no approximations have been made relative to Eq. (1), and Eqs. (3) and (5) are equally difficult to solve. In order to solve

$$\Sigma_{s,1}(u) = \Sigma_{s,1}^{n}(u) + \Sigma_{in,1}(u) \, .$$

while $f_1^1(u' \to u)$ is the scattering energy transfer kernel of isotope i:

$$f_1^1(u' \to u) = \frac{1}{\Sigma_{s,1}^{n}(u')} \left\{ \Sigma_{s,1}^{n}(u') f_{s,1}^{n}(u' \to u) \right.$$

$$\left. + \Sigma_{in,1}(u') f_{in,1}(u' \to u) \right\} \, . \qquad (2)$$

The neutron leakage from a system can be taken into account by adding $B_g^2 \Sigma_{tr}(u)$ to the macroscopic absorption cross section. The subscripts a, f, e, in, and tr refer to absorption, fission, elastic, and inelastic scattering and transport, respectively, and B_g^2 stands for the buckling.

The slowing-down density is defined as:

$$q(u) = \sum_{l} \int_{u-\delta_i^2}^{u} du' \, \Sigma_{s,l}(u') \phi(u') f_l^i(u' \to u) \, du' \, . \qquad (3)$$

Using the identity

$$\frac{dq(u)}{du} = \Sigma_s(u) \phi(u) - \sum_{l} \int_{u}^{u+\delta_i^2} du' \, \Sigma_{s,l}^{i}(u') \phi(u') f_l^i(u' \to u) \, . \qquad (4)$$

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$$\frac{dq(u)}{du} = S(u) - \Sigma_a(u) \phi(u) \, . \qquad (5)$$

Up to this point no approximations have been made relative to Eq. (1), and Eqs. (3) and (5) are equally difficult to solve. In order to solve

Eqs. (3) and (5), conventional GG theory utilizes the feature that the isotopic scattering collision density is a smooth function of lethargy, and makes the Taylor's expansion

$$\Sigma_{s,i}(u')\phi(u') \simeq \Sigma_{s,i}(u)\phi(u) + (u' - u)\frac{d}{du}\left[\Sigma_{s,i}(u)\phi(u)\right] , \qquad (6)$$

while Stacey's I-GG theory utilizes the feature that the total collision density is a smoother function of lethargy, and makes the Taylor's expansion

$$\Sigma_t(u')\phi(u') \simeq \Sigma_t(u)\phi(u) + (u' - u)\frac{d}{du}\left[\Sigma_t(u)\phi(u)\right] . \qquad (7)$$

The validity of such approximations depends upon the composition, and on the lethargy range in question.

Since the total collision density is a more slowly varying quantity than each of the isotopic scattering collision densities, Stacey has succeeded in showing that the I-GG approximation yields significantly better results than the GG approximation in the vicinity of several iron resonances for a typical fast-breeder reactor composition. However, the lethargy increase in inelastic scattering is so large that neither of the above approximations is valid for the inelastic events.

In order to overcome this difficulty, the author proposes a new Taylor's expansion of a more slowly varying quantity, a ratio R(u) of the solution neutron spectrum $\phi(u)$, to the reference spectrum g(u), i.e.

$$R(u')\left[\equiv \phi(u')/g(u')\right] = \sum_{n=0}^{\infty} \frac{(u' - u)^n}{n!} \frac{d^n}{du^n} R(u) . \qquad (8)$$

Eqs. (3) and (5), conventional GG theory utilizes the feature that the isotopic scattering collision density is a smooth function of lethargy, and makes the Taylor's expansion

$$\Sigma_{s,l}(u')\phi(u') \simeq \Sigma_{s,l}(u)\phi(u) + (u' - u)\frac{d}{du}\left[\Sigma_{s,l}(u)\phi(u)\right] . \qquad (6)$$

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In order to overcome this difficulty, the author proposes a new Taylor's expansion of a more slowly varying quantity, a ratio $\Phi(u)$ of the solution neutron spectrum $\psi(u)$, to the reference spectrum $g(u)$, i.e.

$$\Phi(u') \equiv \psi(u')/g(u') \simeq \sum_{n=0}^{\infty} \frac{(u' - u)^n}{n!} \frac{d^n}{du^n} \Phi(u) . \qquad (8)$$

As long as the g(u) is chosen reasonably, the function R(u) can be slowly varying over the slowing-down interval not only in the lower energy range but also in the intermediate and higher energy ranges, where inelastic events are important and where the GG and I-GG approximations have failed.

We can derive a Generalized Goertzel-Greuling (G-GG) theory by the same procedure as was applied in the I-GG theory.

Using Eq. (8) in Eq. (3), we find that

$$q(u) = \sum_i - N_i \sum_{n=0}^{\infty} K_i^n(u) \frac{d^n R(u)}{du^n} , \qquad (9)$$

where $K_i^n(u)$ is defined as

$$K_i^n(u) \equiv - \frac{1}{n!} \int_{u-\Delta_i}^{u} du' \int_{u}^{u'+\Delta_i} du'' \, \sigma_{s,i}(u') g(u') f_i(u' \to u'')(u' - u)^n , \qquad (10)$$

and N_i is the atomic number density of isotope i of the mixture. Differentiation of Eq. (9) yields

$$\frac{dq(u)}{du} = - \sum_i N_i \sum_{n=0}^{\infty} \cdot \left[K_i^n(u) \frac{d^{n+1}}{du^{n+1}} R(u) + \frac{dK_i^n(u)}{du} \frac{d^n R(u)}{du^n} \right] . \qquad (11)$$

Neglecting second and higher derivative terms and combining Eqs. (9) and (11), we get

$$q(u) + \gamma(u) \frac{dq(u)}{du} = - \sum_i N_i \cdot \left[K_i^0(u) + \gamma(u) \frac{dK_i^0(u)}{du} \right] \cdot R(u) , \qquad (12)$$

As long as the $q(u)$ is chosen reasonably, the function $R(u)$ can be slowly varying over the slowing-down interval not only in the lower energy range but also in the intermediate and higher energy ranges, where inelastic events are important and where the 0D and 1-0D approximations have failed.

We can derive a generalized Goertzel-Greuling (G-GG) theory by the same procedure as was applied in the 1-0D theory.

Using Eq. (8) in Eq. (3), we find that

$$q(u) = \sum_{i} - N_i \sum_{n=0} k_n^i(u) \frac{d^n R(u)}{du^n} , \qquad (9)$$

where $k_n^i(u)$ is defined as

$$k_n^i(u) = \frac{1}{n!} \int_{u-\Delta}^{u} du' \int_{u'-\Delta}^{u} du'' \, \sigma_s^{-1}(u'')\sigma(u'')f_i(u''+u''-u')(u'-u)^n , \qquad (10)$$

and N_i is the atomic number density of isotope i of the mixture. Differentiation of Eq. (9) yields

$$\frac{dq(u)}{du} = - \sum_{i} N_i \sum_{n=0} \left[k_n^i(u) \frac{d^{n+1} R(u)}{du^{n+1}} + \frac{dk_n^i(u)}{du} \cdot \frac{d^n R(u)}{du^n} \right] . \qquad (11)$$

Neglecting second and higher derivative terms and combining Eqs. (9) and (11), we get

$$q(u) + \lambda(u) \frac{dq(u)}{du} = - \sum_{i} N_i \left[k_0^i(u) + \lambda(u) \frac{dk_0^i(u)}{du} \right] - R(u) , \qquad (12)$$

where $\gamma(u)$ is defined as

$$\gamma(u) \equiv -\sum_i N_i K_i^1(u) \Big/ \sum_i N_i \left[K_i^0(u) + \frac{dK_i^1(u)}{du} \right] .$$

By introducing the following composite moderating parameters

$$\xi_i(u)^{12} \equiv -K_i^0(u)/g(u) , \qquad a_i(u) \equiv -K_i^1(u)/g(u) ,$$

$$C_i(u)^{12} \equiv -\frac{dK_i^0(u)}{du} \Big/ g(u) , \qquad e_i(u) \equiv \left[K_i^0(u) + \frac{dK_i^1(u)}{du} \right] \Big/ g(u) , \tag{13}$$

we get the GG-type equation:

$$q(u) + \gamma(u) \frac{dq(u)}{du} = \hat{\xi}(u)\phi(u) , \tag{14}$$

where the basic moderating parameters ξ, a, c, and e are defined as sums of isotopic moderating parameters. Thus $\xi(u) \equiv \sum_i N_i \xi_i(u)$, $a(u) \equiv \sum_i N_i a_i(u)$, etc. Further

$$\hat{\xi}(u) = \xi(u) + \gamma(u) \cdot C(u)$$

and (15)

$$\gamma(u) = a(u)/e(u) .$$

When Eq. (5) is used to eliminate the flux $\phi(u)$ in Eq. (14), and the resulting equation is integrated directly, we obtain

where $\gamma(u)$ is defined as

$$\gamma(u) = -\sum_i M^i K_0^i(u) \Big/ \sum_i M^i \left[K_0^i(u) + \frac{dK_0^i(u)}{du} \right]$$

By introducing the following composite moderating parameters

$$\varepsilon^i(u) = -K_0^i(u)/a(u) \, , \qquad a^i(u) = -K_1^i(u)/a(u) \, ,$$

$$c^i(u) = -\frac{dK_0^i(u)}{du} \Big/ a(u) \, , \qquad e^i(u) = \left[K_0^i(u) + \frac{dK_0^i(u)}{du} \right] \Big/ a(u) \, , \tag{13}$$

we get the BE-type equation:

$$a(u) \frac{dq(u)}{du} + \gamma(u) = \varepsilon(u) q(u) \, , \tag{14}$$

where the basic moderating parameters ε, a, c, and e are defined as sums of isotopic moderating parameters. Thus $\varepsilon(u) = \sum_i M^i \varepsilon^i(u)$, $a(u) = \sum_i M^i a^i(u)$, etc. Further

$$\varepsilon(u) = c(u) + \gamma(u) \cdot e(u) \, , \tag{15}$$

and

$$\gamma(u) = a(u)/a(u) \, .$$

When Eq. (9) is used to eliminate the flux $q(u)$ in Eq. (14), and the resulting equation is integrated directly, we obtain

$$q(u) = \exp - \int_0^u du' \frac{\Sigma_a(u')}{M(u')} \left[q(0) + \int_0^u du' \frac{\hat{\xi}(u')}{M(u')} \right.$$

$$\left. \cdot S(u') \exp \int_0^{u'} du'' \frac{\Sigma_a(u'')}{M(u'')} \right] , \qquad (16)$$

where

$$M(u) = \hat{\xi}(u) + \gamma(u)\Sigma_a(u) , \qquad (17)$$

The flux and slowing-down density are related by

$$\phi(u) = [q(u) + \gamma(u)S(u)]/M(u) . \qquad (18)$$

The microscopic moderating parameters ξ_i, a_i, c_i, and e_i defined in Eq. (13) consist of averages over the slowing-down intervals of the individual isotopes of the mixtures, averages with weights $\sigma_{e,i}g(u')$ and $\sigma_{in,i}g(u')$.

When $g(u')$ is taken as $1/\Sigma_t(u')$ over the slowing-down interval, the present approximation for the elastic scattering reduces to the I-GG approximation.[5] When $g(u)$ is redefined to depend upon i and taken as $1/\sigma_{e,i}(u)$ over the slowing-down interval, the elastic moderating parameters ξ_e and γ_e reduce identically to those of the GG approximation[2] except for the absence of the factor $1/\Sigma_e$ in the definition of $\xi_e(u)$:

$$\xi_e(u) = \sum_i \Sigma_{e,i}(u) \left(1 - \frac{\alpha_i \ln 1/\alpha_i}{1 - \alpha_i} \right) ,$$

$$\gamma_e(u) = \left\{ \xi_e(u) - \sum_i \Sigma_{e,i}(u) \cdot \frac{\alpha_i \left[\ln 1/\alpha_i \right]^2}{2 \cdot \left(1 - \alpha_i \right)} \right\} \Big/ \Sigma_e(u) . \qquad (19)$$

Further we find (still taking $g(u) = 1/\sigma_{e,i}(u)$) that $C_e(u) = 0$.

Moreover, in the treatment of inelastic scattering, when $g_i(E)$ is taken as $1/\sigma_{in,\lambda_i}(E)$ and a Taylor's expansion such as Eq. (8) is performed in energy, the moderating parameters $\xi_{in}(E)$ and $\gamma_{in}(E)$ for the inelastic discrete model reduce to those of Segev's[6] approximation, i.e.

$$\xi_{in}(E) = \sum_i \sum_{\lambda_i} \Sigma_{in,\lambda_i}(E) Q_{\lambda_i} ,$$

$$\gamma_{in}(E) = \frac{1}{2} \sum_i \sum_{\lambda_i} \Sigma_{in,\lambda_i}(E) Q_{\lambda_i}^2 \Big/ \sum_i \sum_{\lambda_i} \Sigma_{in,\lambda_i}(E) Q_{\lambda_i} , \qquad (20)$$

and

$$C_{in}(E) = 0 .$$

Here Q_{λ_i} and Σ_{in,λ_i} are, respectively, the excitation energy and the inelastic cross section of the λ-*th* level of the nuclide i, and $\Sigma_{in}(E)$ is equal to $\sum_i \sum_{\lambda_i} \Sigma_{in,\lambda_i}(E)$.

III. NUMERICAL TESTS AND DISCUSSION

A. Computational Procedures and Test Problems

Some numerical calculations have been performed with a lethargy interval of 1/120 to demonstrate the validity of the present theory for an infinite iron medium and typical fast reactor compositions, whose parameters are given in Table I. The problems CO and BL in Table I have, respectively, core and blanket compositions typical of a fast-breeder reactor, and the problem REF has the average number densities of CO and BL with equal weight. Parameters for a core highly enriched in plutonium, designated HIE-CO, are among those listed in Table I. This core has been included in the present

study in order to illustrate the performance of the method for a wide range of reactor parameters.

All the nuclear data in our compositions were processed from ENDF/B-III[13] using the ETOE-2[14] code but, for the sake of simplicity, some were subsequently modified. One modification was in the treatment of the uranium and plutonium absorption cross sections below the unresolved resonance energies. The uranium cross section was changed to a 1/v cross section with a 2200 mps value of 500 b. The plutonium cross section was represented by a 1/v cross section with a 2200 mps value of 900 b superimposed on a constant cross section of 2.5 b. The validity of treating the narrow resonances of heavy isotopes separately from the basic slowing-down calculation has been demonstrated by Stacey.[5] Another modification was made in the inelastic reaction data. Since the aim of this paper is simply to demonstrate the method presented here, inelastic reactions were treated by discrete and simple evaporation models, and limited to (n,n′) reaction. Inelastic and elastic scatterings were assumed to be isotropic in the center of mass system.

The comparison MG calculations were made with the MC^2-2[15] code, in which the same nuclear data as in the CSD theory calculations were used. Henceforth, the CSD theory presented here is referred as the G-GG theory.

Because the present method is based on the assumption that the R(u) is slowly varying, one must choose a reasonable g(u) or Fg(u)[$\equiv g(u) \cdot \Sigma_{tr}(u)$] before carrying out the spectrum calculation. The following three types of Fg(u) were chosen tentatively:

Option 1: $Fg(u) = \int_0^u \chi(u)\, du$.

Option 2: Fg(u) taken from the reference system.

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All the nuclear data in our compositions were processed from ENDF/B-III[13] using the ETOE-2[14] code but, for the sake of simplicity, some were subsequently modified. One modification was in the treatment of the uranium and plutonium absorption cross sections below the unresolved resonance energies. The uranium cross section was changed to a 1/v cross section with a 2200 mps value of 500 b. The plutonium cross section was represented by a 1/v cross section with a 2200 mps value of 300 b superimposed on a constant cross section of 215 b. The validity of treating the narrow resonances of heavy isotopes separately from the basic slowing-down calculation has been demonstrated by Stacey.[2] Another modification was made in the inelastic reaction data. Since the aim of this paper is simply to demonstrate the method presented here, inelastic reactions were treated by discrete and simple evaporation models, and limited to (n,n') reaction. Inelastic and elastic scatterings were assumed to be isotropic in the center of mass system.

The comparison MC calculations were made with the MC²-2[15] code, in which the same nuclear data as in the CSD theory calculations were used. Henceforth, the CSD theory presented here is referred as the λ-CSD theory.

Because the present method is based on the assumption that the $R(u)$ is slowly varying, one must choose a reasonable $q(u)$ or $f_q(u)[= q(u) \cdot \sigma_{t,0}(u)]$ before carrying out the spectrum calculation. The following three types of $f_q(u)$ were chosen tentatively:

Option 1: $f_q(u) = \int_0^u \chi(u)\, du$.

Option 2: $f_q(u)$ taken from the reference system.

Option 3: Fg(u) calculated from Eqs. (16) and (18) by use of a microscopic moderating parameter library. The library parameters are computed in a reference system, using the G-GG theory.

When one has no information on the fine-group spectrum $\phi(u)$, it is necessary to start from Option 1. Since the first solution by the G-GG method may not be sufficiently accurate, we have to iterate once or twice on Fg(u). The convergence being rapid, as will be discussed later, we can get accurate solutions on the second iteration. When some information on moderating parameters or on $\phi(u)$ is available for a reference system, Option 2 or 3 can be applied. The accuracy of the solution depends on how the reference composition differs from the compositions in the particular problem that we want to solve. Below we show, through several demonstrations, that solutions obtained by use of Option 2 or 3, with a reference system designated as "REF" in Table I, agree quite well with MG results for many varieties of core and blanket compositions. In the latter part of this section it is also shown that the g(u) itself, computed via Option 3, agrees well with MG results.

B. Calculational Results and Discussion

Figure 1 demonstrates the convergence of Option 1 of the proposed method. Since the convergence of the iterative process is very rapid, the chaindotted line which corresponds to the collision density at the second iteration lies on the solid line representing the MG collision density. The collision density at the third iteration is not shown in the figure, because it merges with the MG result. The local difference which was observed in a narrow energy range at the second iteration has disappeared by the third iteration.

In Fig. 2 the calculated moderating parameters ξ, ξ_{in}, and γ are compared for the I-GG[16] and G-GG (Option 3) theories in the CO composition, and the resulting spectra are shown in Figs. 3 and 4. Specifically, the Option 3 computation proceeds as follows: First, moderating parameters appropriate to the "REF" composition are taken from a parameter library and inserted into Eqs. (16) and (18). The function $\phi(u)$ is then put into Eq. (13) (in place of g(u)) and the moderating parameters are recomputed. The recalculated parameters are then reinserted into Eqs. (16) and (18), and $\phi(u)$ is recomputed. The corresponding MG result is also shown in Figs. 3 and 4.

As we would expect, large differences are observed between the ξ's of both methods in higher energy ranges in Fig. 2. The ξ and ξ_{in} in the G-GG theory show fluctuations as functions of energy, fluctuations which are due to the fluctuation of the quantity $[1/\Sigma_s(u)]/g(u)$. On the other hand, those moderating parameters in the I-GG theory do not fluctuate because, in this case, g(u) is set equal to $1/\Sigma_t(u)$. The agreement between the G-GG and MG spectra is fairly good over the whole energy range: in contrast the I-GG approximation fails in the high energy range because of the poor approximation for inelastic scattering.

The applicability of the G-GG theory has been checked for many varieties of fast reactor core and blanket compositions, and similar good agreement with MG result has been observed.

In practice the efficiency of the G-GG method is considerably enhanced if it is possible to make use of a precomputed parameter library. Therefore, it is very important to investigate whether spectral calculation can be performed accurately through use of such a library; that is, to determine whether the g(u) given by Option 3 agrees well with the MG spectrum.

Figures 5 and 6 show the calculational results for HIE-CO and BL compositions obtained by use of a single set of microscopic moderating parameters calculated for one reference composition, designated "REF". The functions g(u) from Option 3 are in surprisingly good agreement with MG results. Note that these g(u)'s are obtained by inserting moderating parameters, from a parameter library, directly into Eqs. (16) through (18). Thus, in this case the computation of g(u) does not involve the recalculation of moderating parameters. The good agreement between g(u)'s so obtained, and MG results, suggests a great advantage of G-GG theory relative to the MG method, because in the calculation of g(u) by Option 3, a good deal of nuclear data is preprocessed and need not be treated explicitly. Thus, for example the Option 3 calculation does not make use, explicitly, of inelastic cross sections and Q value for each discrete level, or the nuclear temperatures and cross sections for the statistical model in inelastic events, while the MG calculation does require the processing of such data.

However, we must be aware that it is necessary to iterate on g(u) in the application of this theory to a system where the spectrum shape is completely different from the reference spectrum. For example in an infinite iron reflector, the absorption of the medium is so small that the $\phi(u)$ rarely decreases substantially at large u. Therefore, whether one chooses Option 1, 2, or 3, it is necessary to iterate on g(u). Figure 7 shows the results at the first and third iterations, for an iron reflector, obtained by use of Option 3. It will be seen that good agreement with the MG method can be obtained at the third iteration.

Finally the coarse-group effective microscopic cross sections $\langle \sigma_{t,Fe} \rangle$ and $\langle \sigma_{c,Na} \rangle$ are compared in Table II for various approximations. Cross

sections listed in the column labelled "g(u)" were obtained as follows. First, moderating parameters appropriate to the "REF" composition were inserted into Eqs. (16) and (18). Then the $\phi(u)$ computed from these equations were used in the calculation of the group-collapsed cross sections. The cross sections in the column labelled "G-GG" were computed via Option 3, and the spectrum shown in Fig. 3 is the final spectrum used in the group-collapsing process.

Note that the large errors in the columns labelled "I-GG" are due to the failure of the I-GG approximation in the presence of inelastic scattering. This sort of behavior is to be expected since the I-GG approximation was specifically designed to treat elastic scattering and was never intended for the treatment of inelastic scattering.

SUMMARY

The author has generalized a continuous slowing-down theory so that inelastic scattering can be taken into account accurately. Tests of the present theory show quite good agreement in the neutron spectrum and effective cross sections with multigroup calculations over the whole energy range. It is thus demonstrated that the present theory can be used as an attractive alternative to multigroup theory for the calculations of neutron spectra in fast-reactor compositions.

CSD theory has an evident advantage relative to multigroup theory because inelastic and elastic matrices are not required for the CSD formalism in the slowing-down source calculation. Moreover, it must be emphasized that the success of the utilization of a microscopic moderating parameter library gives a great advantage to the CSD theory, since the

sections listed in the column labelled "$g(u)$" were obtained as follows. First, moderating parameters appropriate to the "REF" composition were inserted into Eqs. (15) and (16). Then the $\xi(u)$ computed from these equations were used in the calculation of the group-collapsed cross sections. The cross sections in the column labelled "C-GA" were computed via Option 5, and the spectrum shown in Fig. 3 is the final spectrum used in the group-collapsing process.

Note that the large errors in the columns labelled "I-GG" are due to the failure of the I-GG approximation in the presence of inelastic scattering. This sort of behavior is to be expected since the I-GG approximation was specifically designed to treat elastic scattering and was never intended for the treatment of inelastic scattering.

SUMMARY

The author has generalized a continuous slowing-down theory so that inelastic scattering can be taken into account accurately. Tests of the present theory show quite good agreement in the neutron spectrum and effective cross sections with multigroup calculations over the whole energy range. It is thus demonstrated that the present theory can be used as an attractive alternative to multigroup theory for the calculations of neutron spectra in fast-reactor compositions.

CSD theory has an evident advantage relative to multigroup theory because inelastic and elastic matrices are not required for the CSD formalism in the slowing-down source calculation. Moreover, it must be emphasized that the success of the utilization of a microscopic moderating parameter library gives a great advantage to the CSD theory, since the

CSD theory yields an accurate neutron spectrum quickly without the use of a vast amount of inelastic data.

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[12]Since $\xi_i(u)$ and $C_i(u)$ include, in their definitions, the pointwise values of g(u) outside the integral sign, a large error in $\xi_i(u)$ and $C_i(u)$ can be anticipated in the case where the pointwise values g(u) differ sharply and erratically from the solution spectrum $\phi(u)$. As long as the global shape of g(u) does not differ so much from that of $\phi(u)$, the pointwise random errors tend to cancel in the integration. By imposing the condition of neutron balance, Eq. (1), on g(u), the pointwise g(u) can be corrected as

$$\tilde{g}(u) = \left\{ S(u) + g(u) \left[\sum_i \Sigma_{s,i}(u) - C(u) \right] \right\} \Big/ \Sigma_t(u) ,$$

where the $\tilde{A}(u)$ stands for the corrected value of A at lethargy u. In the

demonstration calculation for the present theory in Section III, the pointwise value g(u) at u is replaced by $\tilde{g}(u)$ while the integral value is kept unchanged, i.e.

$$\tilde{\xi}(u) = \xi(u)g(u)/\tilde{g}(u) ,$$

$$\tilde{C}(u) = \sum_i \left\{ \Sigma_{s,i} \cdot [\tilde{g}(u) - g(u)] + g(u) \cdot C(u) \right\} \Big/ \tilde{g}(u) .$$

It is clear from Eqs. (14) and (15) that the above correction is not necessary for the parameters a(u) and e(u), because only the ratio of a(u) to e(u) appears in the GG-type equation (14).

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The option of the multigroup approximation was applied in the calculation for the elastic and inelastic events.

[16] It is clear that the I-GG method, as originally developed by Stacey,[5] was designed for the treatment of elastic scattering in spectrum calculations. This method is unsuited to the treatment of inelastic scattering and was never intended for such a purpose. Nevertheless comparisons between the extended I-GG method and the G-GG method seem to be of some interest, and the extended I-GG method was developed specifically to permit such comparisons. Although it may be inappropriate to refer to our extended version of Stacey's method as "I-GG" theory we will, for the sake of convenience, continue to do so.

TABLE I

Parameters Used in Test Computations

I.D. of Problem	HIE-CO	CO	BL	REF	Fe
Fission spectrum	^{239}Pu	^{239}Pu	^{238}U	^{239}Pu	^{239}Pu
$PuO_2/(PuO_2 + UO_2)$, %	25	15	0	5.7	---
Volume Fraction, %					
Fuel	35		60	48	0
Fe	24		16	20	100
Na	41		24	32	0
Buckling B_g^2 (cm^{-2})	0.0018		0.0	0.0009	0

TABLE I

Parameters Used in Test Computations

I.D. of Problem	HIF-CO	CO	BL	CEF	Fe
Fission Spectrum	^{239}Pu	^{239}Pu	^{239}Pu	^{239}Pu	^{239}Pu
$PuO_2/(PuO_2 + UO_2)$, %	25	15	0	5.7	---
Volume Fraction, %					
Fuel	25	60	48	0	
Fe	24	15	20	100	
Na	41	24	32	0	
Buckling B_g^2 (cm^{-2})	0.0018		0.0	0.0009	0

TABLE II

Comparison of Effective Cross Sections in the CO composition

$$D\left(\left\langle \sigma_{x,i} \right\rangle\right) = \frac{\left\langle \sigma_{x,i} \right\rangle - \left\langle \sigma_{x,i,MG} \right\rangle}{\left\langle \sigma_{x,i,MG} \right\rangle} \times 100(\%) \quad (x = t \text{ or } c)^{a}$$

Coarse Group	Lower Energy (E_{max} = 10 MeV)	$\langle \sigma_{t,Fe} \rangle$	$D(\langle \sigma_{t,Fe} \rangle)$, %			$\langle \sigma_{c,Na} \rangle$	$D(\langle \sigma_{c,Na} \rangle)$, %		
		MG (b)	I-GG	g(u)[b]	G-GG[c]	MG (mb)	I-GG	g(u)[b]	G-GG[c]
1	3.68 MeV	3.635	0.0	0.0	0.0	0.163	0.0	0.0	0.0
2	1.35	3.136	0.1	0.1	0.0	0.190	-0.1	-0.1	0.0
3	498. keV	2.600	1.2	0.0	-0.1	0.291	-0.1	0.5	0.3
4	183.	3.020	-6.8	0.1	-0.1	0.588	-2.1	0.2	-0.1
5	67.4	3.521	-20.1	0.2	-0.2	1.053	-11.6	-0.1	0.0
6	24.8	7.163	4.2	-0.4	-0.3	2.374	-4.5	0.1	0.0
7	9.12	2.330	4.0	-0.7	-0.5	0.343	1.1	-0.2	-0.2
8	3.36	9.590	0.3	0.1	0.0	4.834	0.1	-0.6	-0.3
9	1.34	8.050	-0.1	-0.1	0.0	34.23	0.4	0.5	0.5
10	454. eV	9.736	-0.1	0.0	0.0	5.482	0.0	0.0	0.0
11	167.	10.93	0.0	0.0	0.0	8.052	0.0	0.0	0.0
12	61.5	11.41	0.0	0.0	0.0	9.292	-0.1	-0.1	-0.1

[a] $\langle \sigma_{x,i,MG} \rangle$ is the effective cross section of reaction x in element i using the MG approximation (MC^2-2).

$\langle \sigma_{x,i} \rangle_{IG} = \int_{\Delta IG}^{du} \sigma_{x,i}(u)\phi(u) \Big/ \int_{\Delta IG} du\phi(u)$, where IG is coarse group number and ΔIG is the coarse-group width.

[b] Calculated from Eqs. (16) and (18) by use of a set of microscopic moderating parameters from REF composition.

[c] Option 3 is applied.

TABLE II

Comparison of Effective Cross Sections in the CO composition

$$\Delta\left(\langle\sigma_{x,i}\rangle\right) = \frac{\langle\sigma_{x,i,MC}\rangle - \langle\sigma_{x,i}\rangle}{\langle\sigma_{x,i,MC}\rangle} \cdot 100(\%) \quad (x = t \text{ or } c)^a$$

Coarse Group	Lower Energy (E_{max} = 10 MeV)	$\langle\sigma_{t,Fe}\rangle$	$\Delta\left(\langle\sigma_{t,Fe}\rangle\right)$, %		$\langle\sigma_{c,Ni}\rangle$	$\Delta\left(\langle\sigma_{c,Ni}\rangle\right)$, %		
		MG (b)	1-GG	$\sigma(u)^b$	MG (mb)	1-GG	$\sigma(u)^b$	0-GG^c
1	3.68 MeV	3.635	0.0	0.0	0.163	0.0	0.0	0.0
2	1.35	3.738	0.1	0.0	0.190	-0.1	-0.1	0.0
3	498. keV	2.600	1.2	0.0	-0.1	0.291	-0.1	0.8	0.3
4	183.	3.020	-6.8	0.1	-0.1	0.588	-2.1	0.2	-0.1
5	67.4	3.521	-20.1	0.2	-0.2	1.059	-11.6	-0.1	0.8
6	24.8	7.163	4.2	-0.4	-0.3	2.274	-4.5	0.1	0.0
7	9.12	2.230	4.0	-0.7	-0.5	0.343	1.1	-0.2	-0.2
8	3.36	9.590	0.3	0.1	0.0	4.824	0.1	-0.6	-0.3
9	1.34	8.060	-0.1	-0.1	0.0	34.23	0.4	0.8	0.5
10	454. eV	9.758	-0.1	0.0	0.0	5.482	0.0	0.0	0.0
11	167.	10.93	0.0	0.0	0.0	8.052	0.0	0.0	0.0
12	61.5	11.47	0.0	0.0	0.0	3.292	-0.1	-0.1	-0.1

$^a\langle\sigma_{x,i,MC}\rangle$ is the effective cross section of reaction x in element i using the MG approximation (MC²-2).

$\langle\sigma_{x,i}\rangle_{IG} = \left(\int_{\Delta IG} \sigma_{x,i}(u)\varphi(u)\,du(u)\right) / \Delta IG$, where IG is coarse group number and ΔIG is the coarse-group width.

^{b}Calculated from Eqs. (16) and (18) by use of a set of microscopic moderating parameters from REF composition.

^{c}Option 3 is applied.

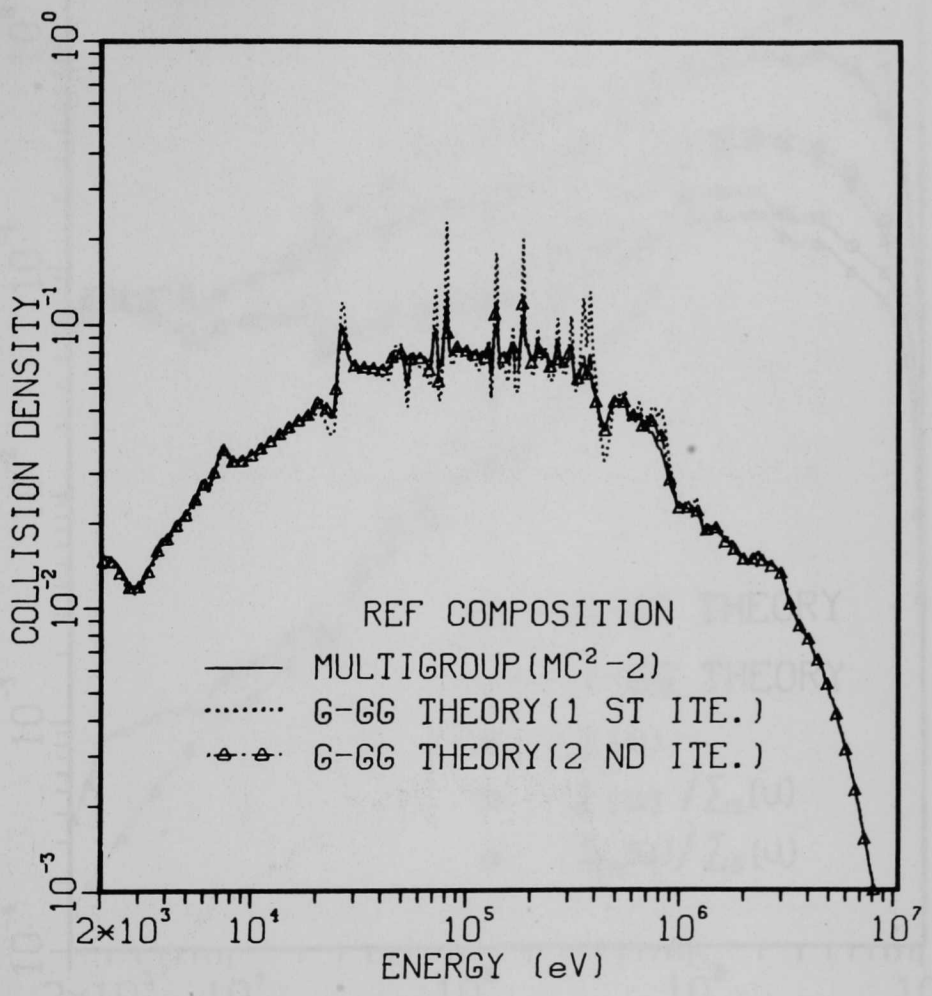
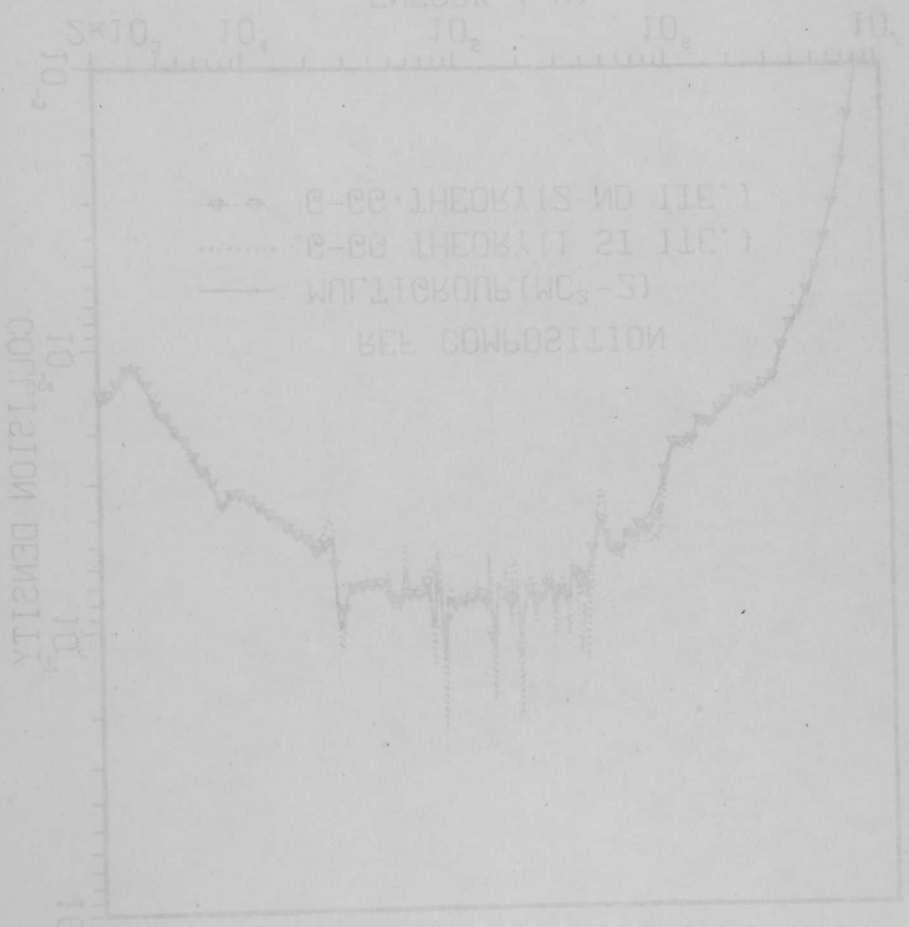


Fig. 1. The convergence of collision densities in the G-GG theory, starting from $g(u) = \int_0^u \chi(u)\, du/\Sigma_{tr}(u)$ in the REF composition.
(ANL Neg. No. 116-2590)


ENERGY (eV)
$5\times10_2$
10_4
10_2
10_3
10_4
10_{-2}
10_{-1}
10_0
10_1
10_2
CORRELATION DENSITY

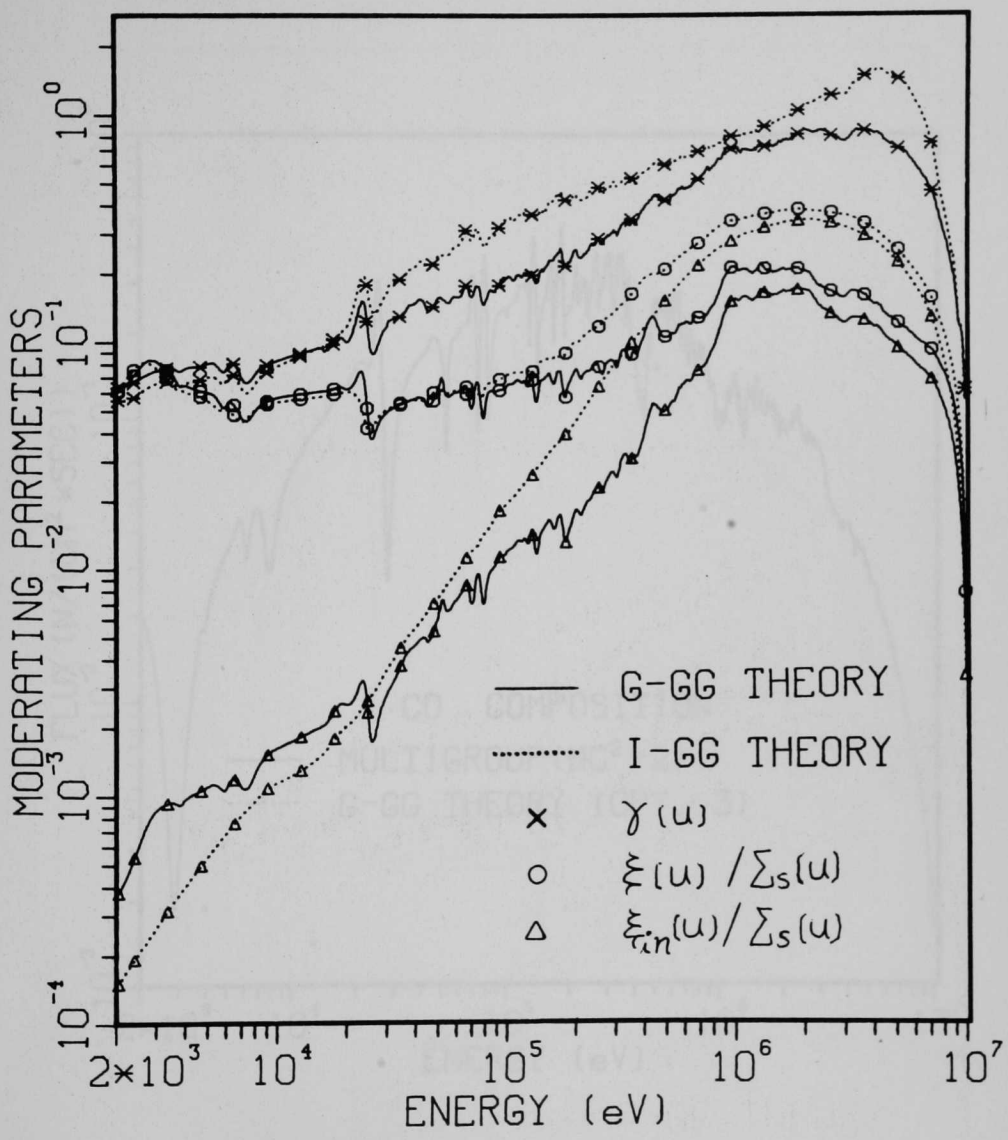
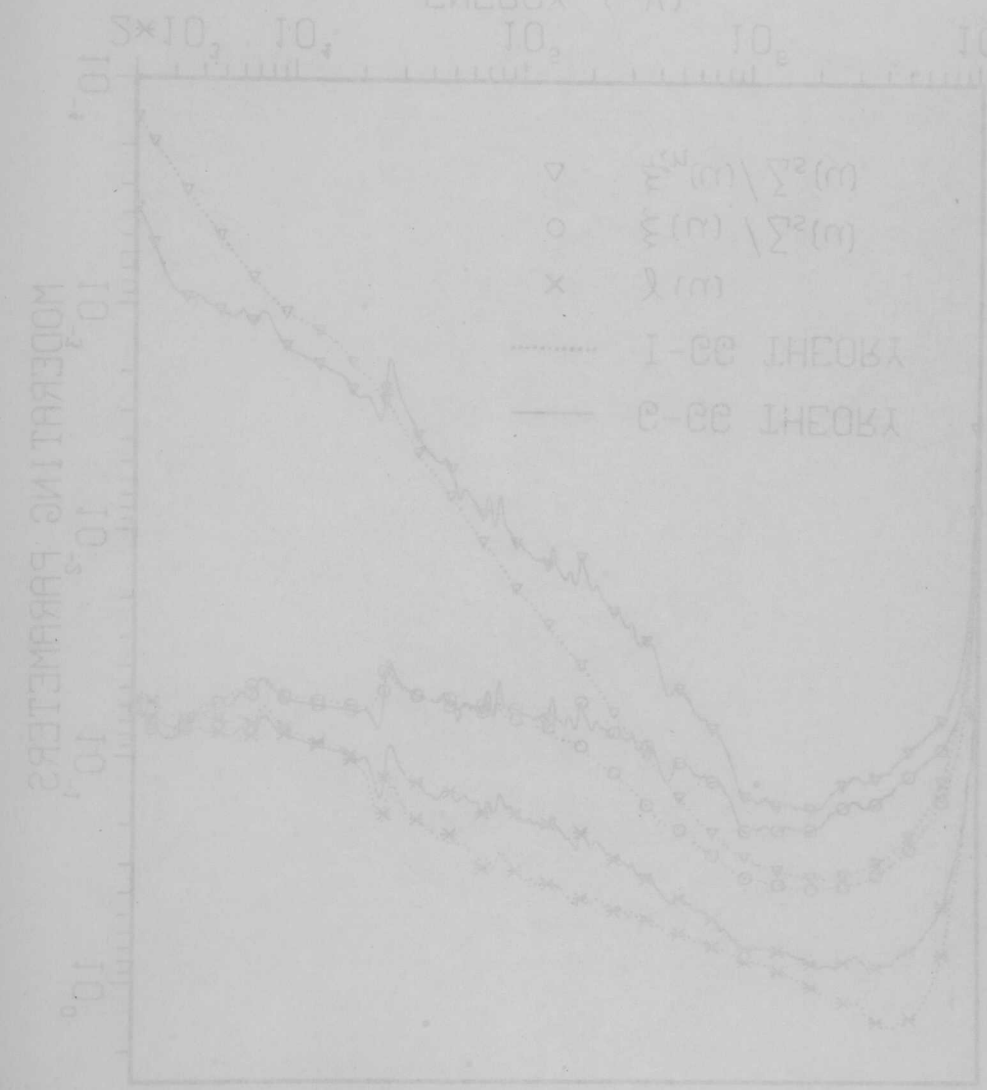


Fig. 2. Comparison between moderating parameters ξ, ξ_{in}, and γ in the I-GG and G-GG theories, and in the CO composition. (ANL Neg. No. 116-2586)


MODE-MIXING PARAMETERS
ENERGY (eV)
$\xi(\omega)$
$\xi(\omega)/\Sigma^2(\omega)$
$\xi^{-1}(\omega)/\Sigma^2(\omega)$
C-CC THEORY
I-CC THEORY

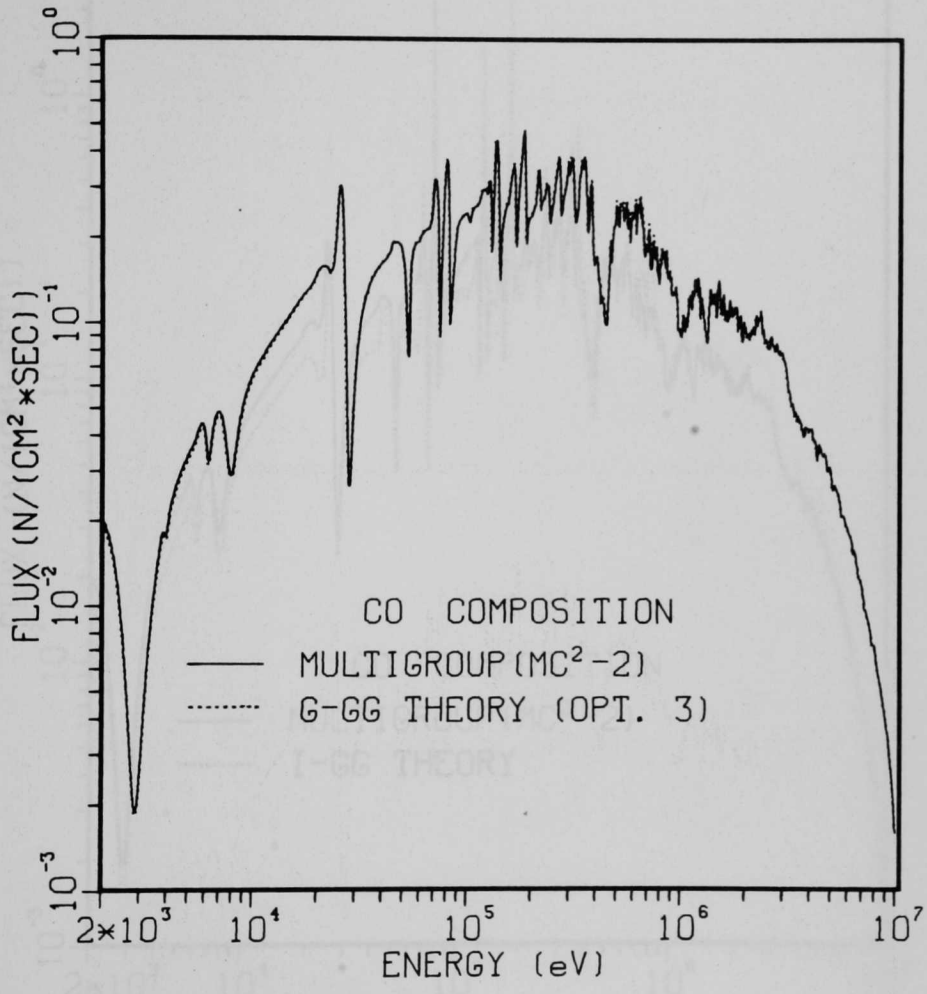


Fig. 3. The G-GG spectrum compared with the MG result in the CO composition. (ANL Neg. No. 116-2589)

Fig. 3. The G-GG spectrum compared with the MG result in the GG composition.
(ANL Neg. No. 116-2589)

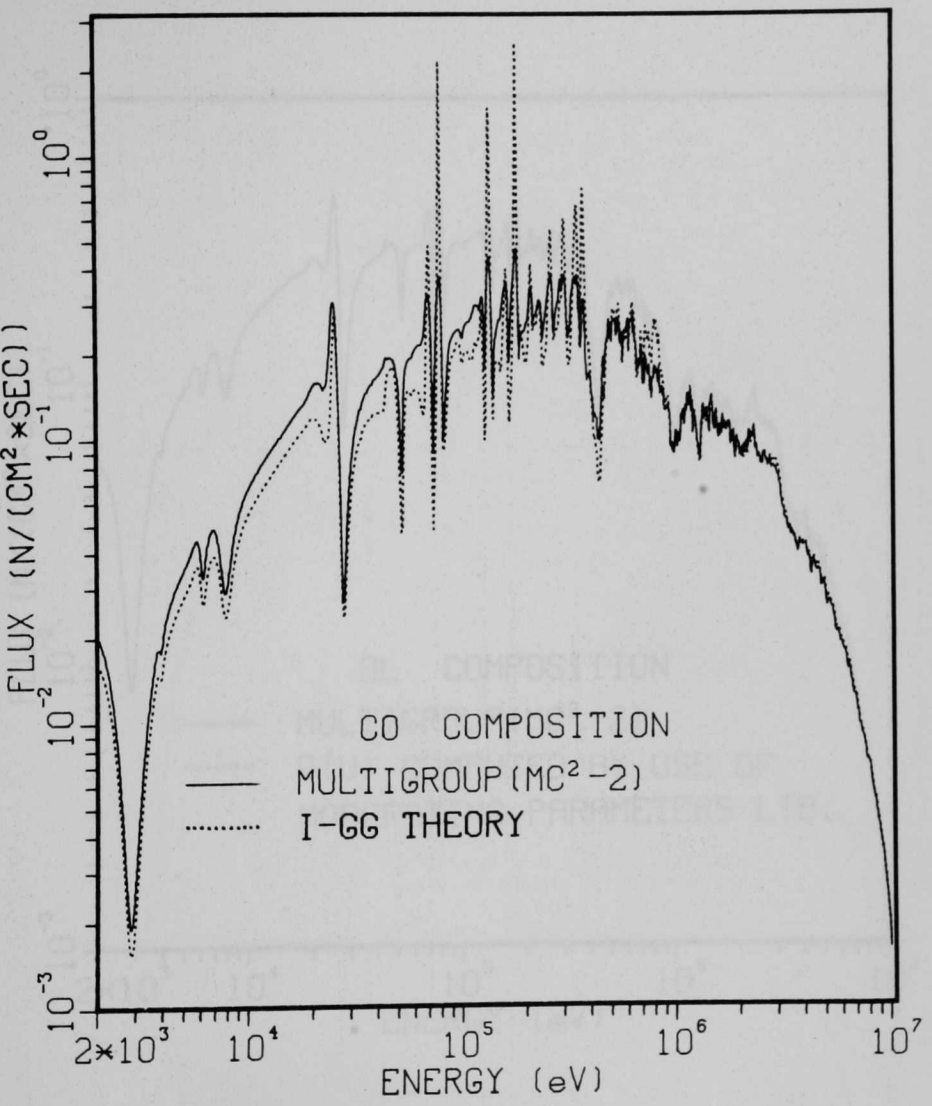


Fig. 4. The I-GG spectrum compared with the MG result in the CO composition. (ANL Neg. No. 116-2585)

Fig. 4. The I-GG spectrum compared with the MG result in the CO composition (ANL Neg. No. 116-2865)

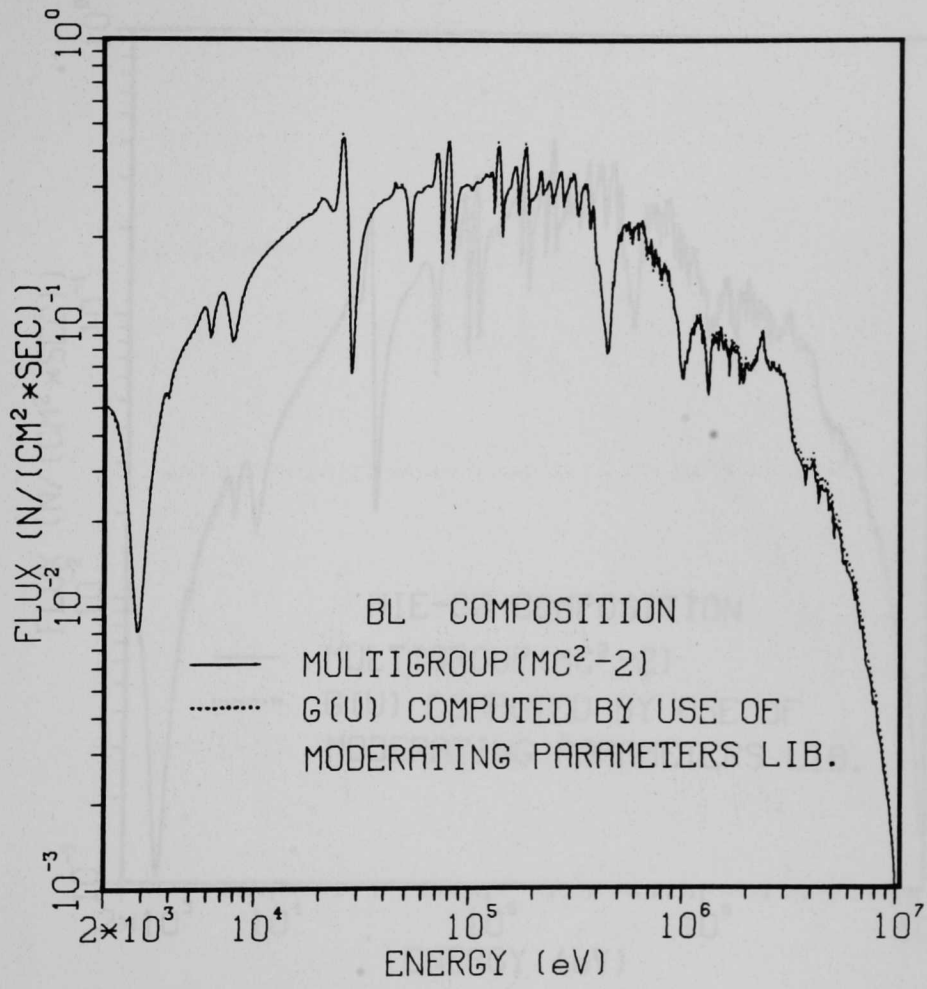


Fig. 5. g(u) in the BL composition, calculated using a set of reference moderating parameters based on G-GG theory.
(ANL Neg. No. 116-2584)

FLUX (N/(CM²×SEC))
ENERGY (eV)
MULTIGROUP(MC²-2)
MODERATING PARAMETERS LIB.

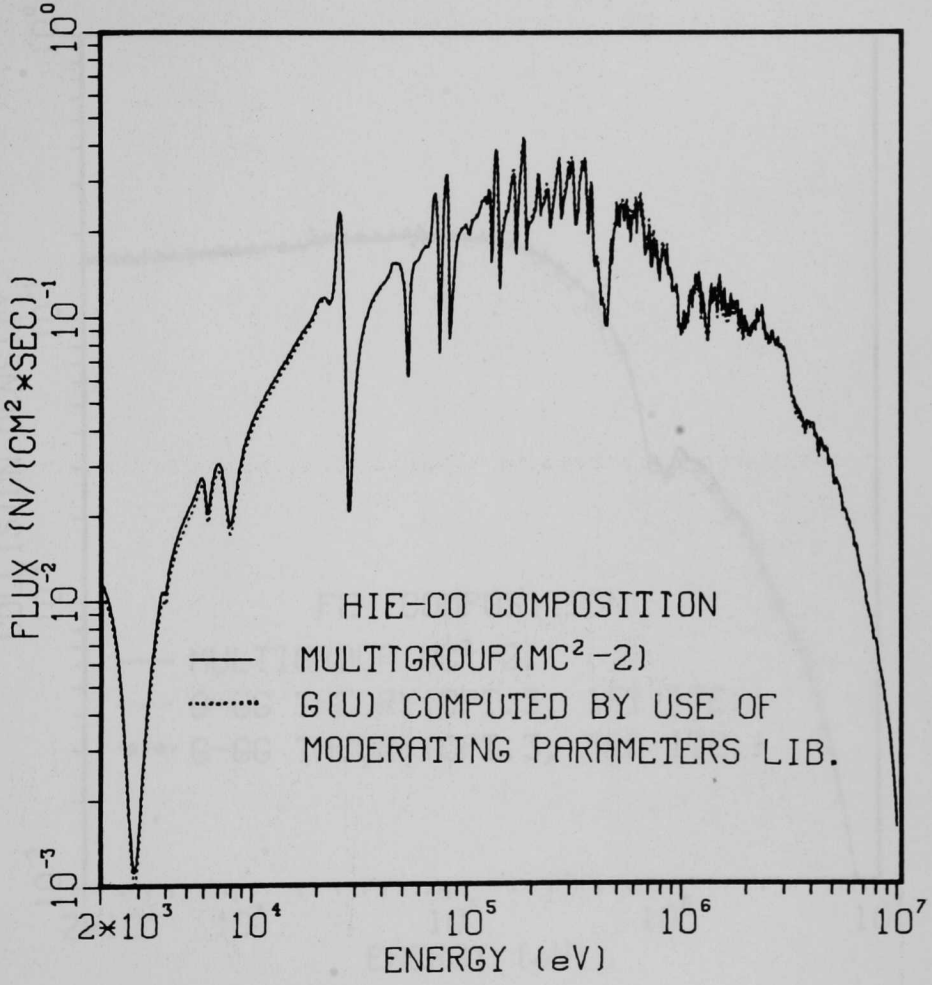


Fig. 6. g(u) in the HIE-CO composition, calculated using a set of reference-moderating parameters based on G-GG theory.
(ANL Neg. No. 116-2587)

10^{0}
10^{-1}
10^{-3}
10^{-5}
FLUX (N/(CM^2 SEC))
2×10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
ENERGY (eV)

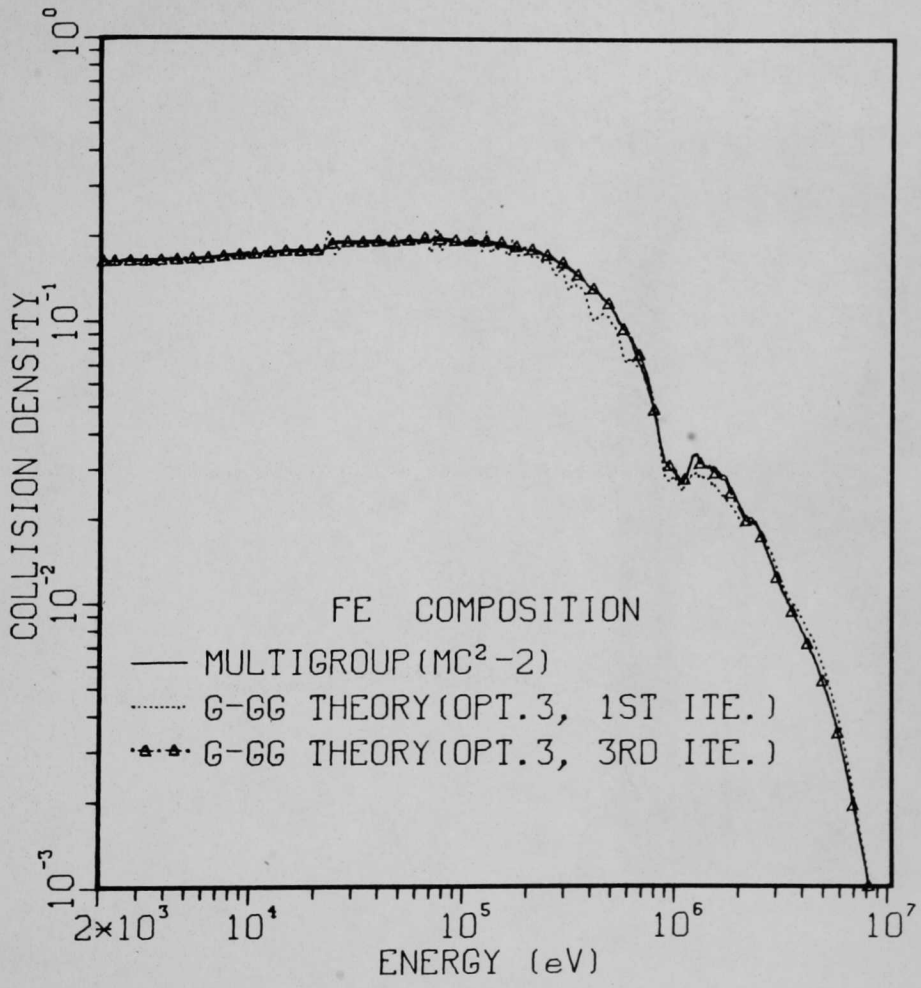
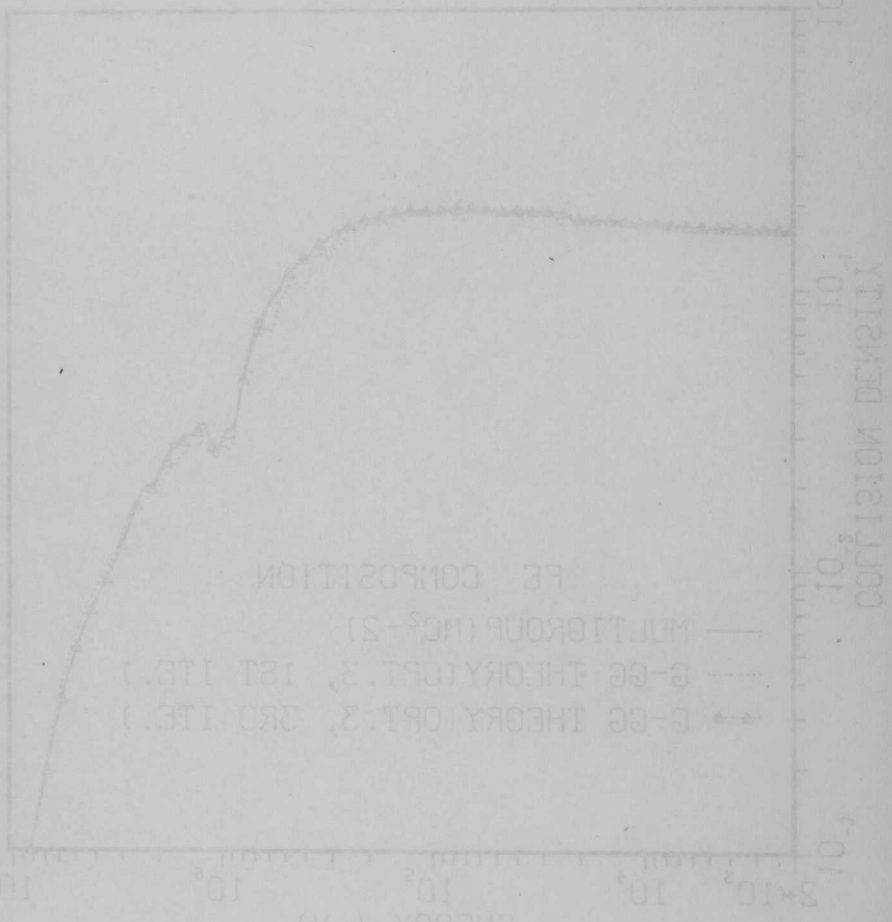


Fig. 7. G-GG collision densities compared with the MG result in an iron reflector. (ANL Neg. No. 116-2591)


COLLISION DENSITY
ENERGY (eV)